

**catena-Poly[[diaquamanganese(II)]- $\mu$ -imino-diacetato- $\kappa^4 O, N, O', O''$ ]****Quan-Zheng Zhang and  
Can-Zhong Lu\***State Key Laboratory of Structural Chemistry,  
Fujian Institute of Research on the Structure of  
Matter, Chinese Academy of Sciences, Fuzhou,  
Fujian 350002, People's Republic of China

Correspondence e-mail: czlu@ms.fjirsm.ac.cn

**Key indicators**

Single-crystal X-ray study

 $T = 293\text{ K}$ Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$ 

H-atom completeness 78%

 $R$  factor = 0.018 $wR$  factor = 0.047

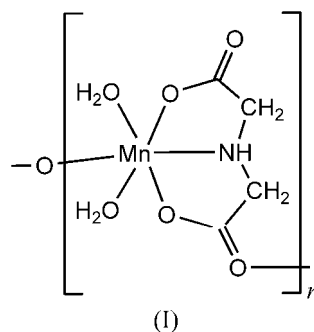
Data-to-parameter ratio = 11.5

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title complex,  $[\text{Mn}(\text{C}_4\text{H}_5\text{NO}_4)(\text{H}_2\text{O})_2]_n$ , the octahedrally coordinated Mn atom is bonded by three carboxyl O atoms, one imino N atom and two water molecules. By means of the bridging iminodiacetate ligand, the title complex exhibits a one-dimensional chain structure, with  $\text{Mn} \cdots \text{Mn}$  distances of 5.362 (1) Å.

**Comment**

As one of the dicarboxylate ligands containing *N*-donors, iminodiacetic acid can act as a potential bifunctional ligand with variable multidentate coordination modes. For instance, a series of iminodiacetate (ida) complexes of Fe (Walters *et al.*, 2003), Co (Junk & Smith, 2002), Ni (Agre *et al.*, 1984) and Cu (Tribet *et al.*, 2003) have been isolated and structurally characterized. Among these complexes, many display polymeric structures in which the ida ligands generally adopt tetra- or pentadentate coordination modes. We report here the synthesis and crystal structure of a polymeric Mn–ida complex, *viz.* catena-poly[[diaquamanganese(II)]- $\mu$ -iminodiacetato], (I).



As shown in Fig. 1, the Mn atom in (I) is coordinated by five O atoms and one N atom; two O atoms are from coordinated water molecules, with Mn–O distances of 2.245 (1) and 2.183 (1) Å, three O atoms are from carboxyl groups, with Mn–O distances of 2.272 (1), 2.155 (1) and 2.122 (1) Å, and the N atom is from the ida ligand, with an Mn–N distance of 2.274 (1) Å (Table 1). The ida ligand displays a tetradentate coordination mode through three carboxyl O atoms (O1, O2 and O3) and the imino N atom. Similar to the reported ida complex of Co (Burshtein & Poznyak, 2000), the title complex exhibits a one-dimensional chain structure (Fig. 2), with  $\text{Mn} \cdots \text{Mn}$  distances of 5.362 (1) Å.

**Experimental**

To a solution of iminodiacetic acid (0.6 mmol),  $\text{MnSO}_4 \cdot \text{H}_2\text{O}$  (0.5 mmol) and  $\text{H}_2\text{O}$  (20 ml) was added an aqueous NaOH solution (1 N) to adjust the pH value to 4–5; ethanol (5 ml) was then added. After stirring for 30 min, the mixture was allowed to stand at room

Received 12 July 2004

Accepted 21 July 2004

Online 31 July 2004

temperature undisturbed for about three weeks, resulting in colorless crystals.

Crystal data

[Mn(C<sub>4</sub>H<sub>5</sub>NO<sub>4</sub>)(H<sub>2</sub>O)<sub>2</sub>]  
*M<sub>r</sub>* = 222.06  
 Orthorhombic, *Pca*2<sub>1</sub>  
*a* = 14.535 (3) Å  
*b* = 5.340 (1) Å  
*c* = 9.731 (2) Å  
*V* = 755.3 (2) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.953 Mg m<sup>-3</sup>

Mo *K*α radiation  
 Cell parameters from 2942 reflections  
 $\theta$  = 2.1–27.5°  
 $\mu$  = 1.74 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Prism, colorless  
 0.37 × 0.23 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.557, *T<sub>max</sub>* = 0.840  
 5189 measured reflections

1536 independent reflections  
 1502 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.016  
 $\theta_{max}$  = 27.5°  
*h* = -18 → 18  
*k* = -6 → 6  
*l* = -12 → 9

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.018  
*wR* (*F*<sup>2</sup>) = 0.047  
*S* = 1.04  
 1536 reflections  
 134 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 ( $\Delta/\sigma$ )<sub>max</sub> = 0.018  
 $\Delta\rho_{max} = 0.44 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.24 \text{ e \AA}^{-3}$   
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.0011 (3)  
 Absolute structure: Flack (1983)  
 Flack parameter = 0.006 (13)

Table 1

Selected geometric parameters (Å, °).

N1—Mn1	2.2738 (14)	Mn1—O6	2.1829 (12)
Mn1—O2 <sup>i</sup>	2.1221 (12)	Mn1—O5	2.2452 (12)
Mn1—O3	2.1547 (12)	Mn1—O1	2.2718 (13)
O2 <sup>i</sup> —Mn1—O3	88.83 (5)	O6—Mn1—O1	158.19 (4)
O2 <sup>i</sup> —Mn1—O6	113.12 (5)	O5—Mn1—O1	83.85 (5)
O3—Mn1—O6	96.37 (5)	O2 <sup>i</sup> —Mn1—N1	155.03 (5)
O2 <sup>i</sup> —Mn1—O5	94.87 (5)	O3—Mn1—N1	77.00 (5)
O3—Mn1—O5	173.82 (5)	O6—Mn1—N1	89.10 (5)
O6—Mn1—O5	86.75 (5)	O5—Mn1—N1	97.76 (4)
O2 <sup>i</sup> —Mn1—O1	87.31 (5)	O1—Mn1—N1	72.80 (5)
O3—Mn1—O1	91.39 (5)		

Symmetry code: (i) 1 - *x*, -*y*, *z* - ½.

The H atom on the N atom was positioned geometrically (N—H = 0.91 Å) and refined as riding, with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(N). H atoms attached to C atoms and the coordinated water atom O6 were located in a difference Fourier map and refined with isotropic displacement parameters. Other H atoms were not located.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

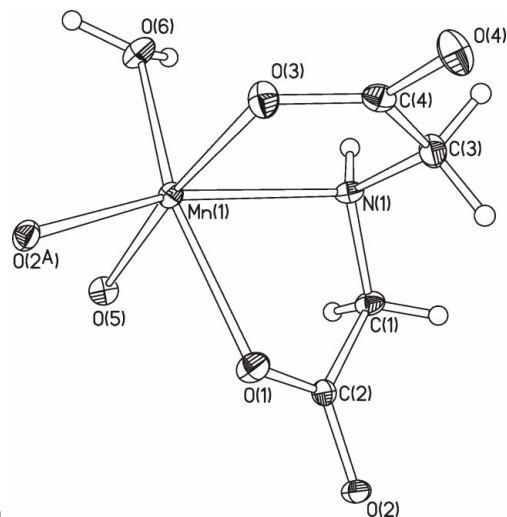


Figure 1  
 A perspective view of the locally expanded unit in (I). Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (A) 1 - *x*, -*y*, *z* - ½].

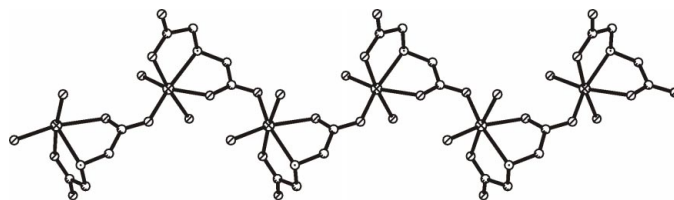


Figure 2  
 The one-dimensional chain structure of (I). H atoms have been omitted for clarity.

*SHELXTL* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

References

Agre, V. M., Sisoeva, T. F., Trunov, V. K., Dyatlova, N. M. & Fridman, A. Y. (1984). *J. Struct. Chem.* **25**, 297–303.  
 Burshtein, I. F. & Poznyak, A. L. (2000). *Crystallogr. Rep.* **45**, 422–423.  
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
 Junk, P. C. & Smith, M. K. (2002). *J. Coord. Chem.* **55**, 1091–1096.  
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.  
 Siemens (1994). *SAINT* and *SHELXTL* (Version 5). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.  
 Siemens (1996). *SMART*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.  
 Tribet, M., Covelo, B., Choquesillo-Lazarte, D., González-Pérez, J. M., Castiñeiras, A. & Niclós-Gutiérrez, J. (2003). *Inorg. Chem. Commun.* **6**, 343–345.  
 Walters, M. A., Vapnyar, V., Bolour, A., Incarvito, C. & Rheingold, A. L. (2003). *Polyhedron*, **22**, 941–946.